

Book Reviews

ACS Symposium series 589

Computer-aided molecular design. Applications in agrochemicals, materials and pharmaceuticals, ed. Charles H. Reynolds, M. Katharine Holloway & Harold K. Cox, American Chemical Society, Washington DC, 1995, x + 428 pages, price US\$109.95. ISBN 0-8412-3160-5

This book reports on a symposium held as part of the 207th national meeting of the American Chemical Society, San Diego, March 1994. The aim of the symposium series is to provide a rapid means of publication and, given that these papers are peer reviewed, this appears to have been achieved for this volume. The contents are evenly divided between agrochemicals, materials and pharmaceuticals and thus about one-third of the volume will be directly relevant to a researcher involved in one of these fields. Some of the topics, however, are of more general interest, for example the effect of tautomeric equilibria on hydrophobicity (A. J. Leo), experimental design in organic synthesis (L. H. Brannigan *et al.*), the use of predictive toxicology in the design of new chemicals (V. K. Gombar and K. Enslein) and the use of genetic algorithms in computer-aided molecular design (V. Venkatasubramanian *et al.*). Other papers which present an example from a particular field contain sufficient information to provide a useful practical guide to particular computational techniques. As a result this volume should be of interest to many who may use computer-aided molecular design (CAMD), whatever their field of work.

The methodology covered in this book is very varied including 'classical' QSAR using regression analysis, 3-D QSAR (CoMFA and HASL), semi-empirical and *ab initio* quantum mechanics calculations, molecular dynamics simulations, multivariate statistics, expert systems and genetic algorithms. The examples are similarly varied and cover theoretical studies of explosives and corrosion, modelling drug diffusion in membranes, the inclusion of metabolism and toxicology in design and the simultaneous analysis of in-vivo and in-vitro data. In the preface the editors highlight a commonly posed question about computer-aided molecular design—'What new products have arisen as a result of CAMD?'. It may be argued that this is not really a

question since the same query is never made about the utility of other tools such as NMR and crystallography. There are, however, sufficient examples shown here to answer this question successfully. One in particular, which illustrates the use of a genetic algorithm for the selection of Human rhinovirus serotypes for compound testing (Jaeger *et al.*), specifically demonstrates the impact of CAMD on the project team.

As the series editor points out in the foreword a book such as this can only provide a 'snapshot in time' of the current state of research on a topic. Some of the techniques described here will have moved on since 1994, particularly the more recent artificial intelligence methods, but the applications of the techniques provide sound examples of the practical use of CAMD. A 'proceedings' volume is always useful to someone who might have attended a conference but was unable to. In the case of this book I have no hesitation in recommending it both to the specialists who apply and develop computer-aided molecular design techniques and to the experimentalists who seek to make use of the methods in their work. These were the two audiences that the editors of this volume had in mind, for both the symposium and the book, and I feel that they have met their target admirably.

D. J. Livingstone

ACS Symposium series 595

Biorational pest control agents—Formulation and delivery, ed. F. R. Hall & J. W. Barry, American Chemical Society, Washington DC, 1995, xii + 306 pp., price US\$84.95.

ISBN 0-8412-3226-1

The aim in the United States of implementing integrated pest management (IPM) on 75% of all agricultural lands by the year 2000 is linked with the aim of reducing pesticide use and of using safer pesticides. In view of these aims, the American Chemical Society sponsored a Symposium on Formulation and Delivery of Biorationals in March 1994. This book provides a wider audience with the papers discussed at the symposium. While many non-conventional pesticide control

tactics had been tried at a laboratory or very small-scale experimental level, the problem of extending their use to practical farm-scale use was identified for a range of biorationals, including *Bacillus thuringiensis*, baculoviruses, pheromones, mycoherbicides and nematodes. After an introductory overview by the editors, the remaining 20 chapters are divided into six sections covering registration needs, basic information needs, delivery and environmental fate, soil biorationals, foliar biorationals and, lastly, forest biorationals.

Registration requirements discussed are principally those in North America. The chapter by R. E. Mickle discusses a generic approach to minimizing impact on non-target species in relation to spray drift with particular reference to aerial applications in forests and highlights the influence of droplet spectra on the resultant buffer zone requirements to protect sensitive environmental areas.

J. R. Fuxa's chapter discusses ecological factors critical to the use of entomopathogens and emphasises the need to understand the crop-pest situations in which biorationals are used. The need to understand the behaviour of the pest in relation to pick-up of the toxin is well illustrated in the following chapter which describes the use of a simulation model to examine the dose transfer of *Bacillus thuringiensis* by diamond back moth larvae on cabbage. Modelling also features in the chapter by M. E. Teske, J. W. Barry and H. W. Thistle who describe their method of spray accountancy in forestry which, combined with ground and water fate models, provides a complete environmental fate prediction system. The forestry system features in the following two chapters (A. and K. Sundaram) which discuss spray distribution and persistence of deposits in relation to *Bt* and an ecdysone agonist, tebufenozide. Also in this section is a short discussion on protection and enhancement of viruses by M. Shapiro. The remaining chapters illustrate the problems of developing formulations suitable for applying biorationals in the soil, on foliage, including biological weed control and concerns about controlling exotic weeds, and in forests. Starch encapsulation is considered to be one of the more promising methods of formulating microbial pesticides. Compared to discussions on formulation, delivery systems are not covered so well, except in terms of modelling dispersal from aerial application.

While the book has a strong emphasis on the situation in North America, the problems of developing safer alternatives to the most toxic conventional insecticides and the problems of pesticide resistance are worldwide. Unfortunately, progress in the use of biorationals in Europe and elsewhere is not covered. It is suggested that there is a need for national leadership and policy to create the environment to adopt biorationals and indicates that in the USA, the National IPM plan provides this framework. However, biorationals are not 'magic bullets' and much needs to be done to improve their

delivery to make them more effective in the real world. This book will therefore provide a most useful digest of information to assist research scientists in their quest for better formulation and application of biorationals. It also contains much information which will be useful to others concerned with delivery of more conventional pesticides. It seems a pity that it has taken so long to produce the book, despite being printed from camera-ready copy.

G. Matthews

Synthesis and chemistry of agrochemicals IV, ed. Don R. Baker, Joseph G. Fenyes & Gregory S. Basarab, American Chemical Society, Washington DC, 1995, xiv + 490 pp., price US\$129.95. ISBN 0 8412 3091 9

This the fourth volume in the symposium series, derived from talks given in the agrochemical division ACS meetings. It consists of no fewer than 40 papers, half of which are devoted to herbicide research, eight to insecticides and the remainder to fungicides.

This volume maintains the high standard set by the first three of the series, with informative and well-presented papers covering a wide range of research. Considering the book is put together from camera-ready manuscripts the quality of reproduction is very high, and random checking showed up very few errors.

The book begins with two overviews, on bioassays and bioisosteres. These provide a stimulating introduction, particularly the former which, although brief, covers a wide range of topics from the importance of bioassays in high throughput screening, to complex aspects such as validation of enzyme targets. These areas, which have impacted strongly on pharmaceutical research, are now clearly set to change the face of agrochemical discovery.

Because this book is in effect proceedings from several conferences, it inevitably gives a selective view of current research, providing snapshots of progress in particular areas. However, the various chapters cover most of the major classes of compound of current interest, and give the reader an accurate view of the latest research. Certainly, read in conjunction with the previous volumes, one would have a comprehensive knowledge of chemical research in the agrochemical world. One minor frustration was that I could not find which symposia the papers in this volume came from, but it appeared that all the papers were received in the autumn of 1994.

This book is very definitely aimed at the specialist researcher, and is not cheap, but with 490 pages it is a valuable addition to the researcher's bookshelves, and is well recommended.

P. J. Crowley